ATOMIC LEVEL STRESS PRODUCTION IN POLYMERIC SYSTEMS

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Stress production in a model monodisperse polymeric material is investigated on multiple scales. The analysis is performed by means of equilibrium and non-equilibrium molecular dynamics. A family of mobile intrinsic coordinate systems is introduced, each system having one axis tied to the end-to-end vector of a generic chain segment of specified length. A similar mobile coordinate system tied to the large semiaxis of the ellipsoidal chains is defined on the chain scale. The atomic level stress is evaluated based on bonded and non-bonded interatomic interactions, and averaged in the global coordinate system, to result in the global, system level stress, and in the various intrinsic systems, to result in the intrinsic stress. The two types of stress are equivalent. It is observed that the deviatoric intrinsic stress is scale independent, a bond, a chain segment and the chain scale intrinsic frame carrying the same stress. The hydrostatic component of the stress tensor scales with the segment length. This concept extends the previously introduced Intrinsic Stress Framework, scale-linking the bond and the chain scales. The dynamics of the system of chains during stress relaxation is described in these various intrinsic frames.